**Amendment to the Claims:**

This listing of claims will replace all prior versions, and listing, of claims in the application.

**Listing of Claims:**

1.      (currently amended) A virtual library of possible combinatorially derived product molecules ~~which can be searched for product molecules having desired properties without the necessity of generating the product structures during the search,~~ generated by the following process:

a)      creating one or more files identifying one or more combinatorial reactions for one or more core structures;

b)      creating separate structural variation files (associated with the reaction identifying files) in which are listed together the structural variations representative of those reactants which will react at each variation site of each combinatorial reaction;

c)      associating with each structural variation, data, characterizing each structural variation including:

1)      characterizing data, taking into account when necessary the structures of the cores with which the structural variations would be combined in the listed combinatorial syntheses, which has not been derived from the application of molecular structural descriptors, validated as possessing a neighborhood property; and

2)    characterizing data, taking into account when necessary the structures of

the cores with which the structural variations would be combined in the

listed combinatorial syntheses, which has been derived from applying

molecular structural descriptors, validated as possessing a neighborhood

property, to the structural variations [.]

wherein the virtual library can be searched for product molecules having desired

properties without the necessity of generating the product structures during the search.

2.    (currently amended) A virtual library of possible combinatorially derived product

molecules ~~which can be searched for product molecules having desired properties without the~~

~~necessity of generating the product structures during the search,~~ generated by the following

process:

a)    creating one or more files identifying one or more combinatorial reactions for one

or more core structures;

b)    creating separate structural variation files (associated with the reaction identifying

files) in which are listed together the structural variations representative of

those reactants which will react at each variation site of each combinatorial

reaction;

c)    associating with each structural variation, data, characterizing each structural

variation including:

(1)    characterizing data, taking into account when necessary the structures of

the cores with which the structural variations would be combined

in the listed combinatorial syntheses which has not been derived from the application of molecular structural descriptors, validated as possessing a neighborhood property; and

(2) characterizing data, taking into account when necessary the structures of the cores with which the structural variations would be combined in the listed combinatorial syntheses, which has been derived from applying molecular structural descriptors, validated as possessing a neighborhood property, to the structural variation; and

d) associating with each core, data characterizing each core including:

(1). characterizing data which has not been derived from application of molecular structural descriptors, validated as possessing a neighborhood property; and

(2) characterizing data which is derived by the following additional steps:

(a) selecting a first core;

(b) selecting an attachment bond on the core;

(c) topomerically aligning the core;

(d) characterizing the core with CoMFA fields and the coordinates of the end points of the other attachment bonds;

(e) repeating steps (b) through (d) for all attachment bonds on the core;

(f) selecting a next core; and

(g) repeating steps (b) through (1') for all cores [.]

wherein the virtual library can be searched for product molecules having desired properties without the necessity of generating the product structures during the search.

3.      (currently amended) A virtual library of possible combinatorially derived product molecules ~~which can be searched for product molecules having desired properties without the necessity of generating the product structures during the search,~~ generated by the following process:

a)      defining chemical transformations and reagents and cores to be used to generate product molecules; and

b)      using appropriate molecular descriptors to precalculate characteristics of the component parts of all possible product molecules [.]

wherein the virtual library can be searched for product molecules having desired properties without the necessity of generating the product structures during the search.

4.      (canceled)

5.      (canceled)

6.      (canceled)

7.      (canceled)

8.      (canceled)

9.      (canceled)

10.     (currently amended) A virtual library of component parts of molecules and their characteristics ~~in which all possible product molecules combinatorially derived from the component parts can be searched, without the necessity of generating the product structures~~

~~during the search, for product molecules having desired properties by searching through only a~~ ~~combination of the descriptors of the component parts of the product molecules,~~ generated by the following process:

a) defining chemical transformations and reagents and cores to be used to specify possible product molecules: and

b) using appropriate molecular descriptors, validated as possessing a neighborhood property, to precalculate characteristics of the component parts of all possible product molecules [.]

<u>wherein all possible product molecules combinatorially derived from the component parts can be searched for, without the necessity of generating the product structures during the search, for product molecules having desired properties by searching through only a combination of the descriptors of the component parts of the product molecules.</u>

11. (currently amended) A virtual library of structural variations, cores, and their associated molecular structural descriptors~~, which can be searched for product molecules derived from the~~ ~~combinatorial assembly of the structural variations and cores having desired properties, by~~ ~~combining descriptors of the structural variations and cores to generate descriptors representative~~ ~~of the product molecules, without the necessity of generating the product structures during the~~ ~~search,~~ generated by the following process:

a) creating one or more files identifying one or more combinatorial reactions for one or more core structures;

b) creating separate structural variation files, associated with the reaction identifying

files, in which are listed together the structural variations representative of those

reactants which will react at each variation site of each combinatorial reaction;

c)   associating with each structural variation, data, characterizing each structural

variation including:

(1)   characterizing data, which has not been derived from applying at least one

molecular structural descriptor, validated as possessing a neighborhood

property, to the structural variations, taking into account when necessary

the structures of the cores with which the structural variations would be

combined in the combinatorial syntheses; and

(2)   characterizing data, which has been derived from applying at least one

molecular structural descriptor, validated as possessing a neighborhood

property, to the structural variations taking into account to the extent

appropriate for application of the descriptor the structures of the cores with

which the structural variation would be combined in the combinatorial

syntheses [.]

wherein the virtual library can be searched for product molecules derived from the

combinatorial assembly of the structural variations and cores having desired properties, by

combining descriptors of the structural variations and cores to generate descriptors representative

of the product molecules, without the necessity of generating the product structures during the

search.

12.   (new) A virtual library of structural variations, cores, and their associated molecular

structural descriptors, ~~which can be searched for product molecules derived from the combinatorial assembly of the structural variations and cores having desired properties, by combining descriptors of the structural variations and cores to generate descriptors representative of the product molecules, without the necessity of generating the product structures during the search,~~ generated by the following process:

    a)    creating one or more files identifying one or more combinatorial reactions for one or more core structures;

    b)    creating separate structural variation files, associated with the reaction identifying files, in which are listed together the structural variations representative of those reactants which will react at each variation site of each combinatorial reaction;

    c)    associating with each structural variation, data, characterizing each structural variation including:

        (1)    characterizing data, which has not been derived from applying at least one molecular structural descriptor, validated as possessing a neighborhood property, to the structural variations, taking into account when necessary the structures of the cores with which the structural variations would be combined in the combinatorial syntheses; and

        (2)    characterizing data, which has been derived from applying at least one molecular structural descriptor, validated as possessing a neighborhood property, to the structural variations taking into account to the extent appropriate for application of the descriptor the structures of the cores with

which the structural variation would be combined in the combinatorial

syntheses; and

d)      associating with each core, data characterizing each core including:

(1).      characterizing data which has not been derived from application of

molecular descriptors, validated as possessing a neighborhood property;

and

(2)      characterizing data which is derived by the following additional steps:

(a)      selecting a first core;

(b).      selecting an attachment bond on the core;

(c)      topomerically aligning the core;

(d)      characterizing the core with CoMFA fields and the coordinates of

the end points of the other attachment bonds;

(e)      repeating steps (b) through (d) for all attachment bonds on the core;

(f)      selecting a next core; and

(g)      repeating steps (b) through (1') for all cores [.]

wherein the virtual library can be searched for product molecules derived from the

combinatorial assembly of the structural variations and cores having desired properties, by

combining descriptors of the structural variations and cores to generate descriptors representative

of the product molecules, without the necessity of generating the product structures during the

search.

13.      (previously presented) A system for identifying from a virtual library of structural

variations, cores, and their associated molecular structural descriptors, product molecules derived

from the combinatorial assembly of the structural variations and cores having desired properties,

without the necessity of generating the product structures during the search, comprising:

    a)    a general purpose <u>programmable digital</u> computer further comprising:

        (1)   ~~input devices~~;

        ~~(2)~~ <u>(1)</u> a central processing unit;

        ~~(3)~~ <u>(2)</u> random access memory;

        ~~(4)~~ <u>(3)</u> additional memory means for storing and accessing data; and

        ~~(5)    output devices;and~~

    b)    a virtual library stored in accessible memory of structural variations, cores, and their associated molecular structural descriptors, which can be searched for product molecules derived from the combinatorial assembly of the structural variations and cores having desired properties, by combining descriptors of the structural variations and cores to generate descriptors representative of the product molecules, without the necessity of generating the product structures during the search, generated by the following process:

        (1)    creating one or more files identifying one or more combinatorial reactions for one or more core structures;

        (2)    creating separate structural variation files, associated with the reaction identifying files, in which are listed together the structural variations representative of those reactants which will react at each

variation site of each combinatorial reaction;

(3)     associating with each structural variation, data, characterizing each

structural variation including:

(a)     characterizing data, which has not been derived from

applying at least one molecular structural descriptor,

validated as possessing a neighborhood property, to the

structural variations, taking into account when necessary

the structures of the cores with which the structural

variations would be combined in the combinatorial

syntheses; and

(b)     characterizing data, which has been derived from applying

at least one molecular structural descriptor, validated as

possessing a neighborhood property, to the structural

variations taking into account to the extent appropriate for

application of the descriptor the structures of the cores with

which the structural variation would be combined in the

combinatorial syntheses.